

SAFETY DATA SHEET

Version 8.4
Revision Date 04/18/2021
Print Date 06/21/2021

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Nitrobenzene
Product Number : 48547
Brand : Supelco
Index-No. : 609-003-00-7
CAS-No. : 98-95-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 1B), H360
Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Blood, H372
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H227 Combustible liquid.
H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled.
H351 Suspected of causing cancer.
H360 May damage fertility or the unborn child.
H372 Causes damage to organs (Blood) through prolonged or repeated exposure if inhaled.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P352 + P312 IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell.
P304 + P340 + P311 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P403 + P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Rapidly absorbed through skin.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₆H₅NO₂
Molecular weight : 123.11 g/mol
CAS-No. : 98-95-3
EC-No. : 202-716-0
Index-No. : 609-003-00-7

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| Component | Classification | Concentration |
|---------------------|--|---------------|
| Nitrobenzene | | |
| | Flam. Liq. 4; Acute Tox. 3; Carc. 2; Repr. 1B; STOT RE 1; Aquatic Acute 3; Aquatic Chronic 3; H227, H301, H331, H311, H351, H360, H372, H402, H412 | <= 100 % |

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Nitrogen oxides (NOx)
Combustible.

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage class (TRGS 510): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

| Component | CAS-No. | Value | Control parameters | Basis |
|--------------|---------|--|------------------------------|---|
| Nitrobenzene | 98-95-3 | TWA | 1 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption | | |
| | | TWA | 1 ppm 5 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | TWA | 1 ppm 5 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | Skin designation | | |
| | | TWA | 1 ppm 5 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | Skin notation | | |
| | | PEL | 1 ppm 5 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

Biological occupational exposure limits

| Component | CAS-No. | Parameters | Value | Biological specimen | Basis |
|--------------|---------|-----------------------------------|---------|---------------------|---|
| Nitrobenzene | 98-95-3 | Methemoglobin | 1.5% Hb | In blood | ACGIH - Biological Exposure Indices (BEI) |
| | Remarks | During or at the end of the shift | | | |

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Nature latex/chloroprene
Minimum layer thickness: 0.6 mm
Break through time: 40 min
Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|--|---|
| a) Appearance | Form: liquid, clear Color: colorless, yellow |
| b) Odor | pungent |
| c) Odor Threshold | No data available |
| d) pH | 8.0 - 8.5 at 1.00000 g/l at 20.0 °C (68.0 °F) |
| e) Melting point/freezing point | Melting point/range: 5 - 6 °C (41 - 43 °F) - lit. |
| f) Initial boiling point and boiling range | 210 - 211 °C 410 - 412 °F - lit. |
| g) Flash point | 88.0 °C (190.4 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, | No data available |

| | | |
|----|--|---|
| | gas) | |
| j) | Upper/lower flammability or explosive limits | Upper explosion limit: 40 %(V) Lower explosion limit: 1.8 %(V) |
| k) | Vapor pressure | 66.7 hPa at 120.0 °C (248.0 °F) 0.3 hPa at 20.0 °C(68.0 °F) |
| l) | Vapor density | No data available |
| m) | Relative density | No data available |
| n) | Water solubility | 1.9 g/l at 20 °C (68 °F) |
| o) | Partition coefficient: n-octanol/water | log Pow: 1.86 at 24.5 °C (76.1 °F) |
| p) | Autoignition temperature | 482.0 °C (899.6 °F) |
| q) | Decomposition temperature | No data available |
| r) | Viscosity | No data available |
| s) | Explosive properties | No data available |
| t) | Oxidizing properties | No data available |

9.2 Other safety information

| | |
|-----------------|--------------------------------|
| Surface tension | 43.4 mN/m at 20.0 °C (68.0 °F) |
|-----------------|--------------------------------|

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents, Strong reducing agents, Strong bases

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 349.0 mg/kg

Remarks: Behavioral: Altered sleep time (including change in righting reflex). Lungs, Thorax, or Respiration: Dyspnea. (RTECS) (Regulation (EC) No 1272/2008, Annex VI)

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LC50 Inhalation - Rat - 4 h - 2.81 mg/l
Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Lacrimation.Behavioral:Tremor.(RTECS)

LD50 Dermal - Rabbit - 760 mg/kg
Remarks: (ECHA)
No data available

Skin corrosion/irritation

Skin - Rabbit
Result: No skin irritation - 24 h
Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation
Remarks: (ECHA)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)

Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: Intraperitoneal injection
Method: OECD Test Guideline 474
Result: negative

Test Type: unscheduled DNA synthesis assay
Species: Rat
Cell type: Liver cells
Application Route: Oral
Method: OECD Test Guideline 486
Result: negative

Carcinogenicity

Suspected of causing cancer.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Nitrobenzene)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Nitrobenzene)

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

May damage fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Inhalation - Causes damage to organs through prolonged or repeated exposure. - Blood

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 28 d - LOAEL (Lowest observed adverse effect level) - 5 mg/kg
Remarks:
(ECHA)

RTECS: DA6475000

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer., Exposure to and/or consumption of alcohol may increase toxic effects.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information**12.1 Toxicity**

| | |
|---|---|
| Toxicity to fish | flow-through test LC50 - Danio rerio (zebra fish) - 92 mg/l - 96 h (OECD Test Guideline 203) |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 35 mg/l - 48 h |
| Toxicity to algae | static test ErC50 - Chlorella pyrenoidosa - 18 mg/l - 96 h (OECD Test Guideline 201) |
| Toxicity to bacteria | static test EC20 - activated sludge - 1,000 mg/l - 30 min (OECD Test Guideline 209) |

12.2 Persistence and degradability

| | |
|------------------|--|
| Biodegradability | aerobic - Exposure time 28 d Result: 50 - 60 % - Readily biodegradable. (OECD Test Guideline 301F) |
|------------------|--|

12.3 Bioaccumulative potential

| | |
|-----------------|--|
| Bioaccumulation | Cyprinus carpio (Carp) - 42 d at 25 °C - 0.125 mg/l(Nitrobenzene) |
|-----------------|--|

Bioconcentration factor (BCF): 3.1 - 4.8
(OECD Test Guideline 305C)

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life with long lasting effects.

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 1662 Class: 6.1 Packing group: II

Proper shipping name: Nitrobenzene

Reportable Quantity (RQ): 1000 lbs

Reportable Quantity (RQ): 1000 lbs

1) Marine pollutant: yes Poison Inhalation Hazard: No

IMDG

UN number: 1662 Class: 6.1 Packing group: II EMS-No: F-A, S-A

Proper shipping name: NITROBENZENE

Marine pollutant : yes

IATA

UN number: 1662 Class: 6.1 Packing group: II

Proper shipping name: Nitrobenzene

SECTION 15: Regulatory information

SARA 302 Components

The following components are subject to reporting levels established by SARA Title III, Section 302:

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| | | |
|--------------|--------------------|-----------------------------|
| Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2008-11-03 |
|--------------|--------------------|-----------------------------|

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

| | | |
|--------------|--------------------|-----------------------------|
| Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2008-11-03 |
|--------------|--------------------|-----------------------------|

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Reportable Quantity : D036 lbs

Massachusetts Right To Know Components

| | | |
|--------------|--------------------|-----------------------------|
| Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2008-11-03 |
|--------------|--------------------|-----------------------------|

Pennsylvania Right To Know Components

| | | |
|--------------|--------------------|-----------------------------|
| Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2008-11-03 |
|--------------|--------------------|-----------------------------|

New Jersey Right To Know Components

| | | |
|--------------|--------------------|-----------------------------|
| Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2008-11-03 |
|--------------|--------------------|-----------------------------|

California Prop. 65 Components

| | | |
|--|--------------------|-----------------------------|
| WARNING! This product contains a chemical known in the State of California to cause cancer. Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2010-06-11 |
|--|--------------------|-----------------------------|

| | | |
|--|--------------------|-----------------------------|
| WARNING: This product contains a chemical known in the State of California to cause birth defects or other reproductive harm. Nitrobenzene | CAS-No. 98-95-3 | Revision Date 2010-06-11 |
|--|--------------------|-----------------------------|

SECTION 16: Other information

Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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